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Abstract

The finite size corrections for the anisotropic Heisenberg model in the gap region are calculated via an exact integral representation based on Bethe ansatz equations (BAE). The energy corrections are determined by saddle point approximation for states without complex roots. The case of symmetric states is discussed in greater detail.

1 Introduction

The calculation of finite size corrections for an exactly integrable model is of interest in at least two directions. On one side, for critical models the energy corrections are closely related to important parameters like central charge or operator dimensions. On the other side, besides its intrinsic interest, the treatment of lattice models for finite but large N can give important insights into finite size studies for both integrable and non-integrable theories.

In this paper we want to study an example of an integrable theory with gap, the anisotropic Heisenberg chain (XXZ) in its antiferromagnetic (non-critical) region.

Despite the fact, that there is up to now no relation between energy corrections for the lowest states and physical interesting parameters, it is worthwhile to examine them in detail. On the one hand, we expect the corrections to be more stable compared to critical region, which makes the use of rather involved techniques like Wiener-Hopf [1, 2] unnecessary. On the other hand, the calculations for excited states via saddle point approximation meet several technical problems to be handled with care.

In sect. 2 we present our definitions, the BAE and their integral representation. Sect. 3 deals with the saddle point approximation for the energy corrections of excited states. In sect. 4 the results are obtained for states without complex roots and in more detail for the symmetric ones among them. Our conclusions are contained in sect. 5.

2 The XXZ model and its BAE

We use the Hamiltonian

$$H = -\frac{1}{2} \sum_{i=1}^N (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z) + \frac{1}{2} N \Delta \quad (2.1)$$

with the parametrization

$$\Delta = -\cosh \gamma \quad (2.2)$$

for $\Delta < -1$.

The BAE take then the form

$$\left(\frac{\sin(\lambda_j + \frac{1}{2}i\gamma)}{\sin(\lambda_j - \frac{1}{2}i\gamma)} \right)^N = - \prod_{k=1}^p \frac{\sin(\lambda_j - \lambda_k + i\gamma)}{\sin(\lambda_j - \lambda_k - i\gamma)}, \quad j = 1 \dots p. \quad (2.3)$$

$|\Re(\lambda_j)| \leq \frac{\pi}{2}$ is limited due to periodicity. The energy per site of a state of p magnons is given by

$$E(N) = -\frac{\sinh^2 \gamma}{N} \sum_{j=1}^p \frac{2}{\cosh \gamma - \cos 2\lambda_j}. \quad (2.4)$$

Following the papers [3] and [4] we introduce the function

$$\phi(z, \alpha) = i \log \left(\frac{\sin(z + i\alpha)}{\sin(z - i\alpha)} \right) \quad (2.5)$$

with its usual cut structure for non-real z . For a real root λ_j the BAE can be rewritten in the form

$$N\phi(\lambda_j, \frac{1}{2}\gamma) = \sum_{k=1}^M \phi(\lambda_j - \lambda_k, \gamma) + \sum_l [\phi(\lambda_j - \xi_l, \gamma) + \phi(\lambda_j - \bar{\xi}_l, \gamma)] + 2\pi I_j, \quad (2.6)$$

where the first sum includes all real roots and the second one includes all complex pairs. For large N they assemble into two-strings

$$\xi = \sigma_c \pm i\frac{\gamma}{2},$$

quartets

$$\xi = \sigma_c \pm i\tau_c, \sigma_c \pm i(\gamma - \tau_c), \quad 0 < \tau_c < \gamma$$

and wide pairs

$$\xi = \sigma_w \pm i\tau_w, \quad \tau_w > \gamma$$

[3].

In the thermodynamic limit $N \rightarrow \infty$ the system (2.6) can be solved easily, when the positions of the complex roots and holes (generated by 'unoccupied' I_h) are fixed.

$$\sigma(\lambda) = \sigma_{\infty}^{\text{vac}}(\lambda) + \frac{1}{N}[\sigma_h(\lambda) + \sigma_c(\lambda) + \sigma_w(\lambda)] \quad (2.7)$$

with

$$\begin{aligned} \sigma_{\infty}^{\text{vac}}(\lambda_i) &= \lim_{N \rightarrow \infty} \left(\frac{1}{N} \frac{dI_i}{d\lambda_i} \right). \\ \sigma_{\infty}^{\text{vac}}(\lambda) &= \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \frac{e^{2im\lambda}}{\cosh(m\gamma)} = \frac{K(k)}{\pi^2} \operatorname{dn} \left(\frac{2K\lambda}{\pi}, k \right) \end{aligned} \quad (2.8)$$

is the density for the ground state. The argument of the elliptic modulus k is given by the relation

$$\frac{K'(k)}{K(k)} = \frac{\gamma}{\pi}. \quad (2.9)$$

The density correction for the holes is given via

$$\sigma_h(\lambda) = \frac{1}{\pi} \sum_{h=1}^{N_h} p(\lambda - \theta_h), \quad (2.10)$$

$$p(\lambda) = \frac{1}{2} + 2 \sum_{m=1}^{\infty} \frac{\cos 2m\lambda}{e^{2m\gamma} + 1}. \quad (2.11)$$

With

$$\sigma_N(\lambda) = \frac{1}{N} \frac{dI}{d\lambda} \equiv \frac{dz_N}{d\lambda} \quad (2.12)$$

one defines an analogue of the thermodynamic density on the basis of the counting function

$$z_N(\lambda) = \frac{1}{2\pi} \left[\phi(\lambda, \frac{1}{2}\gamma) - \frac{1}{N} \sum_{i=1}^p \phi(\lambda - \lambda_i, \gamma) \right] \quad (2.13)$$

for finite N . The appropriate limit is provided by eq. (2.6).

In paper [4] exact integral representations have been derived for this density and the energy $E(N)$:

$$\sigma_N(\lambda) - \sigma_{\infty}(\lambda) = - \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{d\mu}{\pi} p(\lambda - \mu) \times$$

$$\times \left\{ \frac{1}{N} \sum_{i=1}^M \delta(\mu - \lambda_i) + \frac{1}{N} \sum_{h=1}^{N_h} \delta(\mu - \theta_h) - \sigma_N(\mu) \right\}, \quad (2.14)$$

$$E(N) - E_\infty = -2\pi \sinh \gamma \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\lambda \sigma_\infty^{\text{vac}}(\lambda) \left[\frac{1}{N} \sum_{i=1}^M \delta(\lambda - \lambda_i) + \frac{1}{N} \sum_{h=1}^{N_h} \delta(\lambda - \theta_h) - \sigma_N(\lambda) \right]. \quad (2.15)$$

The complex roots have formally dropped out, but one has to keep in mind, that their positions influence the real roots and their holes via BAE.

The formulae (2.14) and (2.15) are the starting point of our analysis.

3 The saddle point approximation

We now consider integrals of the type emerging in eqs. (2.14) and (2.15)

$$I_N = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\lambda f(\lambda) \left[\frac{1}{N} \sum_{i=1}^M \delta(\lambda - \lambda_i) + \frac{1}{N} \sum_{h=1}^{N_h} \delta(\lambda - \theta_h) - \sigma_N(\lambda) \right] \quad (3.1)$$

with a periodic function $f(\lambda + \pi) = f(\lambda)$. With the new variable $z = z_N(\lambda)$ one obtains

$$I_N = \int_0^P dz f(\lambda(z)) \left\{ \frac{1}{N} \sum_{k=1}^{M+N_h} \delta(z - z_k) - 1 \right\} \quad (3.2)$$

with $z_k = \frac{k+\frac{1}{2}}{N}$, $k = 1, 2, \dots, M + N_h = P$.

After the Fourier expansion of the δ -function

$$\frac{1}{N} \sum_{k=1}^{M+N_h} \delta(z - z_k) = \sum_{\alpha=-\infty}^{\infty} (-1)^\alpha e^{2\pi i N z \alpha} \quad (3.3)$$

we write

$$I_N = - \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\lambda f(\lambda) \sigma_N(\lambda) \left\{ \frac{1}{e^{2\pi i N z_N(\lambda-i0)} + 1} + \frac{1}{e^{-2\pi i N z_N(\lambda+i0)} + 1} \right\}$$

$$= \sum_{\substack{\alpha=-\infty \\ \alpha \neq 0}}^{\infty} (-1)^\alpha \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\lambda f(\lambda) \sigma_N(\lambda) e^{2\pi i N \alpha z_N(\lambda)}. \quad (3.4)$$

In that sum every term can be calculated via saddle point approximation for large N , where it is dominated by all solutions of

$$\frac{dz_N}{d\lambda} = \sigma_N(\lambda) = 0 \quad (3.5)$$

in the complex λ -plane.

It is therefore useful to deform the integration contour in representation (3.4) in the following way (s. fig. 1):

$$I_N = - \int_{C_+} \frac{d\lambda f(\lambda) \sigma_N(\lambda) e^{2\pi i N z_N(\lambda)}}{e^{2\pi i N z_N(\lambda)} + 1} - \int_{C_-} \frac{d\lambda f(\lambda) \sigma_N(\lambda) e^{-2\pi i N z_N(\lambda)}}{e^{-2\pi i N z_N(\lambda)} + 1} + \text{pole contributions.} \quad (3.6)$$

Figure 1: The integration contours C_+ and C_- in the complex λ -plane.

The integrals on the two vertical lines cancel each other and the pole contributions result from possible poles in the upper and lower rectangles, respectively (s. below).

Going back to the α -expressions

$$I_N = - \sum_{\alpha=1}^{\infty} \int_{C_+} d\lambda f(\lambda) \sigma_N(\lambda) e^{2\pi i N \alpha z_N(\lambda)} - \sum_{\alpha=1}^{\infty} \int_{C_-} d\lambda f(\lambda) \sigma_N(\lambda) e^{-2\pi i N \alpha z_N(\lambda)} + \text{pole contributions} \quad (3.7)$$

we see that for real $f(\lambda)$ the second term is the complex conjugated of the first, which will now be treated below.

$$\tilde{I}_{N,\alpha} = - \int_{C_+} d\lambda f(\lambda) \sigma_N(\lambda) e^{2\pi i N \alpha z_N(\lambda)}. \quad (3.8)$$

We have shown, that the replacement of σ_N by σ_∞ and z_N by z_∞ causes an error in $\tilde{I}_{N,\alpha}$ of the order $k_1^{\alpha N}$ with $k_1 = ((1 - k')/k)^2$.

In paper [4] integral (3.6) has been calculated (after the replacement above) for the ground state without further approximation, leading to the energy correction

$$E^{vac}(N) - E_\infty^{vac} = - \frac{\sqrt{8k'}}{\pi^{3/2}} K(k) \sinh \gamma \frac{k_1^{N/2}}{N^{3/2}} \left\{ 1 + O\left(\frac{1}{N}\right) \right\}. \quad (3.9)$$

We have repeated the calculations for the ground state in saddle point approximation and quote the main results, because the same method will be used below for excited states, where no analytic procedure can be applied.

The solution of $\sigma_\infty^{vac}(\lambda) = 0$, that is the stationary points, are given by

$$\lambda_0^{vac} = \frac{1}{2}\pi + \frac{1}{2}i\gamma \mod (\pi, i\gamma) \quad (3.10)$$

and we introduce $\lambda_0^\pm = \frac{i\gamma}{2} \pm \frac{\pi}{2}$ for those on the contour C_+ .

Also one has

$$z_\infty^{vac}(\lambda_0^\pm) = \frac{1}{2\pi i} \ln \sqrt{k_1}. \quad (3.11)$$

After standard saddle point approximation technique [5] we obtain the asymptotic expansion for $N \rightarrow \infty$

$$\tilde{I}_{N,\alpha} \sim \frac{1}{2} k_1^{\frac{N\alpha}{2}} \sum_{\nu=0}^{\infty} \frac{\Gamma(\frac{\nu+1}{2})}{(2\pi i N \alpha)^{\frac{\nu+1}{2}}} [a_\nu^{(1)} - (-1)^{\frac{\nu+1}{2}} a_\nu^{(2)}] \quad (3.12)$$

with the coefficients $a_\nu^{(1)}$ and $a_\nu^{(2)}$

$$a_\nu^{(1/2)} = \frac{1}{\nu!} \frac{d^\nu}{d\lambda^\nu} \left\{ f(\lambda) \sigma_\infty^{vac}(\lambda) \left(\frac{\lambda - \lambda_0^\mp}{\mp \sqrt{\mp(z_\infty^{vac}(\lambda_0^\mp) - z_\infty^{vac}(\lambda))}} \right)^{\nu+1} \right\} \Big|_{\lambda=\lambda_0^\mp}. \quad (3.13)$$

The dominant contribution comes from the term with $\alpha = 1$, so we will neglect the others with higher α .

For the energy from relation (2.15) the result (3.9) follows where the first non-vanishing correction is from $\nu = 2$. Up to now the pole contributions from eq. (3.6) have been neglected. Using

$$\sigma_N(\lambda) \frac{e^{2\pi i N z_N(\lambda)}}{e^{2\pi i N z_N(\lambda)} + 1} = \frac{1}{2\pi i N} \frac{d}{d\lambda} \log(1 + e^{2\pi i N z_N(\lambda)}) \quad (3.14)$$

and the definition of $z_N(\lambda)$ one gets from the BAE poles from all complex roots with $\Im(\xi_i) < \frac{\gamma}{2}$. Their residua are given by

$$\begin{aligned} 2\pi i \operatorname{res}_{\xi_i} \left(\sigma_N(\lambda) \frac{e^{2\pi i N z_N(\lambda)}}{e^{2\pi i N z_N(\lambda)} + 1} \right) &= \oint_{\xi_i} d\lambda \sigma_N(\lambda) \frac{e^{2\pi i N z_N(\lambda)}}{e^{2\pi i N z_N(\lambda)} + 1} \\ &= \frac{1}{2\pi i N} \oint_{-1} dy \frac{1}{1+y} \\ &= \frac{1}{N}. \end{aligned} \quad (3.15)$$

From the numerator in eq. (3.14) we have another kind of poles at $\lambda = \xi_k + i\gamma$ for all complex ξ_k with $\Im(\xi_k + i\gamma) < \frac{\gamma}{2}$, having residua $-\frac{1}{N}$. Thus, only the close roots contribute which for large N group in quartets. The pole contributions in eq. (3.6) are therefore given by

$$\frac{1}{N} \sum_{l,k} (f(\xi_l) - f(\xi_k + i\gamma)). \quad (3.16)$$

Taking into account the formation of quartets we are left with the deviations from exact quartet structure for finite N . A detailed analysis of those terms can be given only after the corrections to the higher level BAE have been found. This fact motivates that we restrict our analysis to states without complex roots.

We now go back to eq. (3.8) with $N = \infty$ and consider at first general excited states. $z_\infty(\lambda)$ is no longer equal to $z_\infty^{vac}(\lambda)$ but has corrections according to

$$z_\infty(\lambda) = z_\infty^{vac} + \frac{1}{2\pi N} \left[\sum_{h=1}^{N_h} \phi(\lambda - \theta_h, \gamma) - \sum_l \{ \phi(\lambda - \xi_l, \gamma) + \phi(\lambda - \bar{\xi}_l, \gamma) \} \right. \\ \left. - \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} (\sigma_h(\mu) + \sigma_c(\mu) + \sigma_w(\mu)) \phi(\lambda - \mu, \gamma) d\mu \right]. \quad (3.17)$$

With the notation

$$h(\lambda) = i \left[\sum_{h=1}^{N_h} \phi(\lambda - \theta_h, \gamma) - \sum_l \{ \phi(\lambda - \xi_l, \gamma) + \phi(\lambda - \bar{\xi}_l, \gamma) \} \right. \\ \left. - \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} (\sigma_h(\mu) + \sigma_c(\mu) + \sigma_w(\mu)) \phi(\lambda - \mu, \gamma) d\mu \right] \quad (3.18)$$

we can rewrite (3.8)

$$\tilde{I}_{N,\alpha} = - \int_{C_+} d\lambda f(\lambda) \sigma_\infty(\lambda) e^{2\pi i N \alpha z_\infty^{vac}(\lambda) + \alpha h(\lambda)} + O(k_1^{\alpha N}) \\ = - \int_{C_+} d\lambda f(\lambda) e^{\alpha h(\lambda)} \sigma_\infty(\lambda) e^{2\pi i N \alpha z_\infty^{vac}(\lambda)} + O(k_1^{\alpha N}). \quad (3.19)$$

Thus this integral can be treated by our former method based on the saddle points of $z_\infty^{vac}(\lambda)$ with the replacement $f(\lambda) \rightarrow f(\lambda) e^{h(\lambda)}$ if $e^{h(\lambda)}$ is holomorphic in a region containing C_+ . Furthermore, $\sigma_\infty(\lambda)$ includes now terms depending on N which must be included in the analysis. We have checked that all those requirements are fulfilled.

4 Energy corrections for states with real roots

As motivated above we consider states without complex roots, holes in the real root distribution are the only excitations left. We analyze the analytical properties of $\sigma_h(\lambda)$ defined through eqs. (2.10) and (2.11). With the definitions

$$z_1 = e^{-2\gamma + 2i\lambda},$$

$$\begin{aligned}
z_2 &= e^{-2\gamma-2i\lambda}, \\
q &= e^{-2\gamma}, \quad 0 < |q| < 1
\end{aligned} \tag{4.1}$$

we derive

$$p(\lambda) = -\frac{1}{2} + \frac{1}{2}[{}_2\Phi_1(q, -1, -q; q, z_1) + {}_2\Phi_1(q, -1, -q; q, z_2)] \tag{4.2}$$

where ${}_2\Phi_1(a_1, a_2, b_1; q, z)$ is the q -analogue of the well-known hypergeometric function ${}_2\Phi_1(a_1, a_2, b_1; z)$ [6]. We need only the case

$${}_2\Phi_1(q, -1, -q; q, -z) = 1 + 2 \sum_{m=1}^{\infty} \frac{z^m}{1+q^m}. \tag{4.3}$$

The analytic properties of those basic hypergeometric series are found in [7]. From there it follows that $\sigma_h(\lambda)$ is a holomorphic function in the region of integration.

Now we can write down for the energy correction

$$\begin{aligned}
E(N) - E_{\infty} &= 2\pi \sinh \gamma \int_{C_+} d\lambda (\sigma_{\infty}^{vac}(\lambda))^2 e^{h(\lambda)} e^{2\pi i N z_{\infty}^{vac}(\lambda)} \\
&\quad + \frac{2\pi \sinh \gamma}{N} \int_{C_+} d\lambda \sigma_{\infty}^{vac}(\lambda) \sigma_h(\lambda) e^{h(\lambda)} e^{2\pi i N z_{\infty}^{vac}(\lambda)} \\
&\quad + \text{c.c.} + O(k_1^N).
\end{aligned} \tag{4.4}$$

To produce an expression like (3.12) we use (3.13) for the general coefficients. For those of the first term in eq. (4.4) we obtain

$$\begin{aligned}
\tilde{a}_{\nu}^{(1/2)} &= \frac{1}{\nu!} \frac{d^{\nu}}{d\lambda^{\nu}} \left\{ (\sigma_{\infty}^{vac}(\lambda))^2 e^{h(\lambda)} \left(\frac{\lambda - \lambda_0^{\mp}}{\mp \sqrt{\mp(z_{\infty}^{vac}(\lambda_0^{\mp}) - z_{\infty}^{vac}(\lambda))}} \right)^{\nu+1} \right\} \Big|_{\lambda=\lambda_0^{\mp}} \\
&= \frac{1}{\nu!} \sum_{i=0}^{\nu} a_{\nu}^{(1/2)} \frac{d^{\nu-i}}{d\lambda^{\nu-i}} \left\{ e^{h(\lambda)} \left(\frac{\lambda - \lambda_0^{\mp}}{\mp \sqrt{\mp(z_{\infty}^{vac}(\lambda_0^{\mp}) - z_{\infty}^{vac}(\lambda))}} \right)^{\nu-i} \right\} \Big|_{\lambda=\lambda_0^{\mp}} \tag{4.5}
\end{aligned}$$

where in the last line $a_{\nu}^{(1/2)}$ are the coefficients for the ground state which have been calculated before. The leading contribution is given by $\nu = 2$ with

$\tilde{a}_2^{(1/2)} = e^{h(\lambda_0^-)} a_2^{(1/2)}$ and causes a term of order $k_1^{N/2} N^{-3/2}$. The analysis of the second term in eq. (4.4) gives a leading behaviour of order $k_1^{N/2} N^{-5/2}$ confirming the superficial analysis that those terms are suppressed by $\frac{1}{N}$.

Hence

$$\begin{aligned} E(N) - E_\infty &= 2\pi \sinh \gamma \frac{1}{2} (a_2^{(1)} e^{h(\lambda_0^-)} + a_2^{(2)} e^{h(\lambda_0^+)}) \frac{k_1^{N/2}}{(2\pi i N)^{3/2}} + \text{c.c.} + O\left(\frac{k_1^N}{N^{5/2}}\right) \\ &= -\frac{\sqrt{8k'}}{\pi^{3/2}} K(k) \sinh \gamma \frac{k_1^{N/2}}{N^{3/2}} \left\{ e^{h(\lambda_0^-)} + \overline{e^{h(\lambda_0^-)}} + O\left(\frac{1}{N}\right) \right\}. \end{aligned} \quad (4.6)$$

Finally we calculate $e^{h(\lambda_0^-)}$. Recalling eq. (3.18) we have

$$\exp(h(\lambda)) = \prod_{h=1}^{N_h} \exp(\tilde{h}(\lambda, \theta_h)), \quad (4.7)$$

$$\tilde{h}(\lambda, \theta_h) = i \left[\phi(\lambda - \theta_h) - \frac{1}{\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} p(\mu - \theta_h) \phi(\lambda - \mu) d\mu \right]. \quad (4.8)$$

It is straightforward to expand in Fourier series

$$\begin{aligned} \tilde{h}(\lambda, \theta_h) &= i \sum_{m=-\infty}^{\infty} c_m(y, \gamma) \frac{e^{2|m|\gamma}}{e^{2|m|\gamma} + 1} e^{2im(x - \theta_h)} \\ c_m(y, \gamma) &= \begin{cases} \frac{i}{m} ((-1)^m - e^{-2m\gamma} e^{-2|m|\gamma}) & : m \neq 0 \\ \pi + 2iy & : m = 0 \end{cases} \end{aligned} \quad (4.9)$$

for $\lambda = x + iy$.

Further for $\lambda = \lambda_0^- = -\frac{\pi}{2} + \frac{i\gamma}{2}$ one has

$$\tilde{h}(\lambda_0^-, \theta_h) = 2F_3(\theta_h) - \frac{\gamma}{2} + i \left[\frac{\pi}{2} + 2F_1(\theta_h) + 2F_2(\theta_h) \right] \quad (4.10)$$

with the new functions

$$\begin{aligned} F_1(\theta_h) &= \sum_{m=1}^{\infty} \frac{1}{m} \frac{e^{2m\gamma}}{e^{2m\gamma} + 1} \sin 2m\theta_h, \\ F_2(\theta_h) &= \sum_{m=1}^{\infty} \frac{(-1)^m}{m} \frac{\cosh m\gamma}{e^{2m\gamma} + 1} \sin 2m\theta_h, \\ F_3(\theta_h) &= \sum_{m=1}^{\infty} \frac{(-1)^m}{m} \frac{\sinh m\gamma}{e^{2m\gamma} + 1} \cos 2m\theta_h. \end{aligned} \quad (4.11)$$

To our knowledge only F_2 is related to known functions [8]:

$$F_2(x) = -\frac{1}{2} \arctan \left(\frac{e^{-\gamma} \sin 2x}{1 + e^{-\gamma} \cos 2x} \right). \quad (4.12)$$

Thus

$$\begin{aligned} \exp(h(\lambda_0^-)) + \overline{\exp(h(\lambda_0^-))} &= 2(-1)^{N_h/2} \exp \left(-\frac{N_h}{2} \gamma \right) \exp \left(2 \sum_{h=1}^{N_h} F_3(\theta_h) \right) \times \\ &\times \cos \left(\sum_{h=1}^{N_h} [F_1(\theta_h) + F_2(\theta_h)] \right). \end{aligned} \quad (4.13)$$

Together with eq. (4.6) this gives the final answer to our problem, the leading energy correction for states with an arbitrary distribution of holes.

Making the result more transparent we consider low excitations ($N_h = 2$) and symmetric states ($\theta_1 = -\theta_2$). The odd functions F_1 and F_2 drop out, we are left with the even function $F_3(\theta)$, $0 \leq \theta \leq \frac{\pi}{2}$, which will be analyzed below. For those states we have obtained

$$E(N) - E_\infty = \frac{\sqrt{8k'}}{\pi^{3/2}} K(k) \sinh \gamma \frac{k_1^{N/2}}{N^{3/2}} \left\{ 2e^{-\gamma} \exp(4F_3(\theta)) + O\left(\frac{1}{N}\right) \right\}. \quad (4.14)$$

With the help of formula (4.3) $F_3(\theta)$ can be given through integrals of basic hypergeometric series

$$\begin{aligned} F_3(\theta) &= \frac{1}{8z_1} \int_0^{z_1} {}_2\Phi_1(q, -1, -q; q, z) dz - \frac{1}{8z_2} \int_0^{z_2} {}_2\Phi_1(q, -1, -q; q, z) dz \\ &\quad + \frac{1}{8z_3} \int_0^{z_3} {}_2\Phi_1(q, -1, -q; q, z) dz - \frac{1}{8z_4} \int_0^{z_4} {}_2\Phi_1(q, -1, -q; q, z) dz, \\ z_1 &= -e^{-\gamma+2i\theta}, \\ z_2 &= -e^{-3\gamma+2i\theta}, \\ z_3 &= -e^{-\gamma-2i\theta}, \\ z_4 &= -e^{-3\gamma-2i\theta}, \\ q &= e^{-2\gamma}, \quad 0 < |q| < 1. \end{aligned} \quad (4.15)$$

F_3 is therefore analytic as long as $|z_i| < 1$ and $\gamma > 0$.

For its asymptotic behaviour with respect to γ it is easier to use formula (4.11). For large γ one can read off

$$F_3(\theta) = -\frac{1}{2}e^{-\gamma} \cos 2\theta + O(e^{-2\gamma}). \quad (4.16)$$

At $\gamma \rightarrow 0$ we expect singularities near the phase transition point because of the vanishing gap, where our method of calculation breaks down. We propose a regularization $m\gamma \rightarrow m\gamma e^{-\epsilon m} = \beta$ and expand in a series of β . This yields an asymptotic expansion of the form

$$F_3(\theta) = \sum_{k=1}^{\infty} a_k \gamma^k \lim_{\epsilon \rightarrow 0} \sum_{m=1}^{\infty} (-1)^m m^{k-1} e^{-\epsilon m k} \cos 2m\theta. \quad (4.17)$$

For small k the coefficients a_k can be determined explicitly [9] and

$$F_3(\theta) = -\frac{1}{4}\gamma + \frac{1}{4} \left(\frac{1}{1 + \cos 2\theta} \right) \gamma^2 + O(\gamma^3). \quad (4.18)$$

We have calculated numerically the functions $F_3(\theta)$ for different γ . The results are shown in figures 2-4.

Figure 2: The function $F_3(\theta)$ for $0 \leq \theta \leq \frac{\pi}{2}$ and different γ .

Figure 3: The same as figure 2 for small γ .

Figure 4: The same as figure 2 for large γ .

From figures 3 and 4 one can see that F_3 is close to its asymptotics except, of course, for the region $\gamma \sim 1$. In general, the whole function becomes more and more flat with increasing γ .

Both effects can also be seen from figure 5, where we show F_3 as function of γ for fixed θ .

Figure 5: The function $F_3(\theta)$ as function of γ for $\gamma > 0$ and fixed values of θ .

The last figure shows that the general structure in the γ - θ -plane is rather involved. With the asymptotics of $F_3(\theta)$ it is straightforward to look at the behaviour of the energy correction in eq. (4.14) for both limits.

For $\gamma \rightarrow \infty$

$$E(N) - E_\infty = \sqrt{\frac{2}{\pi}} (2e^{-\frac{1}{2}})^N \frac{1}{N^{3/2}} \{1 - 2e^{-\gamma} \cos 2\theta + \text{h.o.c.}\} \quad (4.19)$$

and for $\gamma \rightarrow 0$

$$E(N) - E_\infty = 4\sqrt{2\pi} e^{-\frac{\gamma^2}{\gamma}} \frac{1}{N^{3/2}} \left\{ 1 - \gamma + \frac{1}{1 + \cos 2\theta} \gamma^2 + \text{h.o.c.} \right\}. \quad (4.20)$$

The last formula is only valid for $N \rightarrow \infty$ in the way that $k_1^{N/2}$ can still be neglected. That is just what we expect for smaller γ ; one needs larger and larger N to select the leading term.

5 Conclusions

We have calculated the finite size energy corrections for the anisotropic Heisenberg chain (XXZ) in the antiferromagnetic (non-critical) region for weakly excited states. The main result is, that this correction is qualitatively of the same value in order of N as for the ground state. The dependence on the hole parameters can be factorized (formulae (4.6) and (4.13)) and includes besides a general factor (depending on N_h) an oscillating and an exponential factor. Both factors are given through non-elementary functions described by Fourier series.

We have demonstrated that in the gap-region the saddle point approximation works well but has to be treated with care. For states with complex roots we cannot exclude the influence of pole terms, which can be handled only after the corrections to higher level BAE are calculated .

The corrections arising from the fact, that for finite N the hole parameters θ_h cannot be fixed arbitrarily but are discrete numbers separated by $O(\frac{1}{N})$ have not been taken into account. Due to analyticity with respect to θ_h they produce next-to-leading corrections to those calculated above.

References

- [1] Woynarovich F and Eckle H P 1987 J. Phys. A: Math. Gen. **20** L97
- [2] Hamer C J, Quispel G R W and Batchelor M T 1987 J. Phys. A: Math. Gen. **20** 5677
- [3] Babelon O, de Vega H J and Viallet C M 1983 Nucl. Phys. **B220** [FS8] 13
- [4] de Vega H J and Woynarovich F 1985 Nucl. Phys. **B251** [FS13] 439
- [5] Doetsch G 1971 Handbuch der Laplace-Transformation vol. 1-3 Birkhäuser Verlag Basel and Stuttgart
- [6] Bateman H and Erdelyi A 1955 Higher transcendental functions MacGraw-Hill New York
- [7] Gasper G and Rahman M 1990 Basic hypergeometric series Cambridge University Press
- [8] Gradshteyn I S and Ryzhik I M 1981 Summen-, Produkt-, und Integraltafeln Harry Deutsch Thun and Frankfurt/M.
- [9] Meißner S 1994 Finite-Size-Korrekturen zu schwach angeregten Zuständen des antiferromagnetischen Heisenberg-Modells
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